

Critical behavior of the geometrical spin clusters and interfaces in the two-dimensional thermalized bond Ising model

S. Davatolhagh,¹ M. Moshfeghian¹ and A. A. Saberi^{2,3}

¹Department of Physics, College of Sciences, Shiraz University, Shiraz 71454, Iran

²Institut für Theoretische Physik, Universität Zu Köln, Zùlpiche Str. 77, 50937 Köln, Germany

³School of Physics, Institute for Research in Fundamental Sciences (IPM), PO Box 19395-5531, Tehran, Iran

E-mail: davatolhagh@susc.ac.ir

Abstract. The fractal dimensions and the percolation exponents of the geometrical spin clusters of like sign at criticality, are obtained numerically for an Ising model with temperature-dependent annealed bond dilution, also known as the thermalized bond Ising model (TBIM), in two dimensions. For this purpose, a modified Wolff single-cluster Monte Carlo simulation is used to generate equilibrium spin configurations on square lattices in the critical region. A tie-breaking rule is employed to identify non-intersecting spin cluster boundaries along the edges of the dual lattice. The values obtained for the fractal dimensions of the spanning geometrical clusters D_c , and their interfaces D_I , are in perfect agreement with those reported for the standard two-dimensional ferromagnetic Ising model. Furthermore, the variance of the winding angles, results in a diffusivity $\kappa = 3$ for the two-dimensional thermalized bond Ising model, thus placing it in the universality class of the regular Ising model. A finite-size scaling analysis of the largest geometrical clusters, results in a reliable estimation of the critical percolation exponents for the geometrical clusters in the limit of an infinite lattice size. The percolation exponents thus obtained, are also found to be consistent with those reported for the regular Ising model. These consistencies are explained in terms of the Fisher renormalization relations, which express the thermodynamic critical exponents of systems with annealed bond dilution in terms of those of the regular model system.

keywords: Stochastic Loewner evolution, Critical exponents and amplitudes (theory), Classical Monte Carlo simulations

1. Introduction

It is well known that the geometrical spin clusters (i.e., the clusters composed of the neighboring spins of the same sign), undergo a percolation transition at the thermodynamic critical temperature T_c in the two-dimensional Ising model [1]. This type of behavior is believed to be generally valid for a variety of two-dimensional critical models that undergo a continuous phase transition such as the q -state Potts model ($q \leq 4$) [2], which is a q -state generalization of the Ising model ($q = 2$) [3]. The formation of spanning spin clusters and their characteristic percolation exponents, can also be used to characterize the universality class of the corresponding thermal phase transition. Furthermore, at the critical point, the spanning cluster is a scale-invariant fractal object whose fractal dimensions uniquely specify the universality class of the associated continuous phase transition [4].

The critical behavior of a great number of statistical models in two spatial dimensions, has been investigated by the conformal field theory [5]. The conformal invariance property, refers to the invariance under coordinate transformations through which the angles between the crossing lines in the z -plane do not change. From this point of view, the cluster boundaries in the two-dimensional critical systems are considered as conformally invariant curves, and different characteristics such as their fractal dimensions are obtained. Indeed the fractal geometry is a useful mathematical tool for the characterization of a great many complex configurations. Self-similarity is the most important characteristic of such fractal objects. It is well known that the most widely studied statistical models in the condensed matter physics such as the Ising model, its q -state generalization the Potts model at criticality as well as the many critical geometrical phenomena exhibited by the various percolation models, consist of fractal lines [4, 6, 7, 8, 9, 10].

More recently, the spin cluster boundaries (interfaces) in the two-dimensional critical models, have been investigated rigorously using the method of Stochastic Loewner Evolution (SLE), in which the motion of a random walker along the cluster boundary in the upper-half complex plane in the continuum limit is specified by the Loewner dynamics

$$\frac{\partial g_t(z)}{\partial t} = \frac{2}{g_t(z) - \zeta_t}, \quad (1)$$

which contains a Brownian term $\zeta_t = \sqrt{\kappa}B_t$ whose amplitude is given by the SLE parameter κ , also known as the diffusivity [11]. The function g_t maps a parametric curve γ_t in the upper-half complex plane onto the real axis. Thus, given a real function ζ_t and using the initial condition $g_0 = z$, the Loewner differential equation (1) determines the corresponding trace γ_t in the upper-half z -plane. The larger the diffusivity, κ , the more is the deviation from a straight line. Indeed the nature of the SLE traces change

with the diffusivity: for the range of values $0 \leq \kappa < 4$ —a range that includes $\kappa = 3$ characterizing the boundaries of the geometrical clusters (of like sign) in the critical two-dimensional Ising model—the SLE traces are nonintersecting simple curves, while for $4 \leq \kappa \leq 8$ the curves possess double points with possible self-touching (but no crossing), and for $\kappa > 8$ they become space-filling [11, 12, 13]. Thus, the critical fractal dimension of the interfaces D_I introduced by this theory are model dependent. The relation between D_I and κ is given by $D_I = 1 + \frac{\kappa}{8}$ [14]. The exact values are $\kappa = 3$ and $D_I = \frac{11}{8}$ for the geometric spin cluster boundaries of the two-dimensional regular Ising model, as obtained analytically through various methods [15]. Like the thermodynamic critical exponents in statistical mechanics, κ can divide different models into universality classes [13]. The main difference between κ and the thermal critical exponents, is due to the method of definition—one being thermodynamic and the other geometrical in nature. Normally, the characterization of the universality class, requires a minimum of two thermodynamic critical exponents. We note that in the case of two-dimensional critical systems, a single parameter, κ , appears to be sufficient to specify the universality class. This may be attributed to the fact that of the two specifications of the model that significantly influence its critical behavior, i.e. space dimensions d and the order parameter dimensions n , one is held fixed at $d = 2$. Hence, the SLE diffusivity κ alone can be used to specify the universality class of the two-dimensional critical systems.

In the following we focus on the thermalized bond Ising model (TBIM) in two dimensions and investigate the behavior of its geometrical spin clusters (i.e., spin clusters of like sign) and their external boundaries (interfaces) at criticality. A Wolff single-cluster Monte Carlo algorithm is used to generate configurations at and near the criticality on square lattices, and a tie-breaking rule is used to identify non-intersecting geometrical cluster boundaries along the edges of the dual lattice. The rest of this paper is organized as follows. In section 2, the thermalized-bond Ising model is briefly reviewed, focussing on its thermodynamic critical behavior. The method of simulation and the finite size scaling procedures—employed to extrapolate the results obtained for finite lattices to the thermodynamic limit—are explained in section 3. The results are presented and discussed in section 4, and the paper is concluded with a summary in section 5.

2. The model system

The thermalized bond Ising model (TBIM), is a bond-diluted Ising model with a temperature dependent bond concentration, in which every covalent bond linking a nearest neighbor pair of atoms is allowed thermally induced electronic transitions between bonding and anti bonding electronic states [16]. Hence, it can be regarded as containing *annealed* bond defects with a temperature dependent concentration. Each bond at every instant is characterized by a coupling constant $J_{ij} = 0, J_0$, such that zero corresponds to a broken bond (anti-bonding electronic state), while J_0 means an attractive coupling between the two atoms (bonding electronic state), as illustrated

schematically in figure 1. Denoting the thermally averaged bond concentration by p_b , $(1 - p_b)$ must therefore represent the concentration of the broken bonds due to thermal excitations. To keep the analysis simple, the covalent bonds are treated as independent two-level systems with energy gap J_0 , as sketched in figure 1 [16]. The ratio of the bonds to the broken bonds in equilibrium, is given by the ratio of the corresponding Boltzmann factors $p_b/(1 - p_b) = \exp(\beta J_0)$, or

$$p_b = 1/(1 + e^{-\beta J_0}) \quad (2)$$

where $\beta = 1/k_B T$ is the reciprocal temperature and k_B is the Boltzmann constant. The bond distribution function for the thermalized-bond model system is of the form

$$P_{J_{ij}}(\beta) = p_b \delta_{J_{ij}, J_0} + (1 - p_b) \delta_{J_{ij}, 0} \quad (3)$$

where, p_b is given by equation (2), and δ denotes the Kronecker delta [17]. Hence, the Hamiltonian of the system can be formally defined by

$$H = \sum_{\langle i, j \rangle} J_{ij} S_i S_j \quad (4)$$

where $S_i = \pm 1$ is an Ising spin, and the sum is over all nearest-neighbor pairs.

It is well known that mapping the regular Ising model onto the equivalent correlated percolation problem introduces the bond probability

$$P_r = 1 - e^{-2\beta J} \quad (5)$$

for the critical droplets (the Fortuin-Kastelyn clusters) of the regular Ising model [1, 18]. The combination of equation (2) and equation (5), together with the choice $J_0 = 2J$, which is also the energy gap between parallel and antiparallel spins in the regular Ising model, results in a compound bond probability $P_{\text{TBIM}} = P_r p_b$ for our thermalized-bond model system:

$$P_{\text{TBIM}} = (1 - e^{-2\beta J})/(1 + e^{-2\beta J}) = \tanh(\beta J). \quad (6)$$

Equation (6) represents the bond probability used in our single-cluster update MC simulations.

The thermodynamic critical behavior of the TBIM, has been studied before in two [19], and three dimensions [16]. In two dimensions, the critical temperature is estimated to be $T_c = 1.4897(3)$ [19], which is lower than the critical temperature of the regular Ising model. The lowering of the transition point is expected in the light of the annealed bond disorder present. However, the thermal critical exponents are found to be unchanged, within statistical errors. As for the three-dimensional TBIM, the thermal critical exponents are found to change consistent with the Fisher renormalization relations, as the specific heat exponent of the regular Ising model in three dimensions, $\alpha_r \simeq 0.11$, is finite and positive.

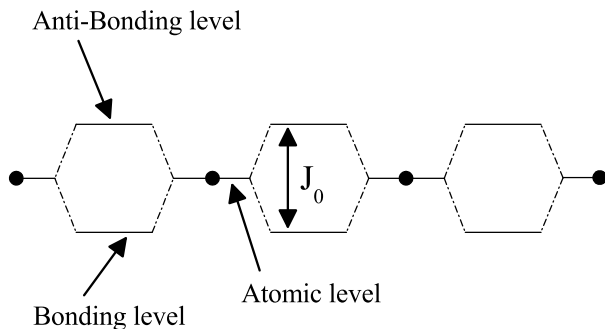


Figure 1. Schematic illustration of the electronic energy states of the covalent bonds linking a chain of atoms. The energy gap between the bonding and the antibonding level is denoted by J_0 .

3. Simulation method and finite-size scaling

As pointed out in the introduction, the critical behavior of the geometrical spin clusters and interfaces in the two-dimensional TBIM, is the main goal of this paper. For consistency with the postulates of SLE at T_c , we have considered the model on strips of size $L_x \times L_y$, where the length of the strip L_x is taken to be much larger than its width $L_y = L$ with an aspect ratio $L_x/L_y = 8$. The boundary conditions used for simulations, are fixed for the lower boundary (real axis), antiperiodic for the two sides, and free for the upper boundary of the system, as shown schematically in figure 2. Using a single-cluster update algorithm (Wolff's algorithm) [20] for the two-dimensional TBIM on square lattice, we generated equilibrium spin configurations at and near the critical point T_c . A typical run consisted of several weeks of the CPU time on a single processor computer. Initially, the system was allowed $2 \times 10^3 L$ equilibration Monte Carlo steps (MCS), and then the data points were accumulated by averaging over $2 \times 10^2 L$ configurations that contained a spanning cluster extending along the width of the strip L . Thus, L sets the appropriate length scale for the systems used, and the critical interfaces can be studied by the theory of SLE in the scaling limit. A turn right (or, alternatively, left) tie-breaking rule [21], is used on the square lattice as a procedure to identify the external perimeters (hulls) of the geometrical spin clusters without any self-intersection. We note that in this case the hulls and the external perimeters are the same. To identify the interfaces in the upper half complex plane, a walker moves along the edges of the dual lattice, starting from the origin as sketched in figure 2. At the first step of the walk, a spin (+) lies to the right of the walker (this direction is chosen to be the preferable direction). After arriving at each site on the dual lattice there are 3 possibilities for the walker: it can cross any of the 3 nearest bonds of the original lattice. At the first step of selection, it chooses the bonds containing two different spins where crossing each of them leaves the spin (+) to the right and (−) to the left of walker. The direction right or left are defined locally according to the orientation of the walker. If

there are still two possibilities for crossing, the walker chooses the bond which accords with the turn right tie-breaking rule. It turns toward the bond which is on its right-bond side with respect to its last direction in the last walk, if there is no selected bond to its right, it prefers to move straight on and if there is also no one there, it turns to its left. The procedure is repeated iteratively until the walker touches the upper boundary. The resulting interface is a unique one which has no self-intersection and never gets trapped [21]. Note that we just take the samples including a vertical spanning cluster in the y -direction. The fractal dimension of the interfaces at criticality, D_I , is obtained using the standard finite-size scaling procedure. The length of interfaces is related to the sample size as

$$l \propto L^{D_I}. \quad (7)$$

Indeed the fractal dimension of the conformally invariant curves is provided by the SLE theory as

$$D_I = 1 + \frac{\kappa}{8} \quad (8)$$

in which diffusivity κ , as mentioned in the introduction, characterizes different universality classes, and so does D_I . For the regular Ising model, the diffusivity is believed to be $\kappa = 3$, and thus $D_I = \frac{11}{8} = 1.375$. In addition, the fractal dimension of the spanning spin cluster at T_c , obeys the relation

$$M \propto L^{D_c} \quad (9)$$

where M is the mass of the cluster, and obtained by counting all the nearest-neighbor positive (negative) spins to the right (left) of the SLE trace, as shown in figure 2. The exact value of D_c for the regular Ising model is $D_c = \frac{187}{96} = 1.9479...$ [22]. Besides these, we find the winding angle variance through the winding angle function $w(e)$ as defined by Wilson and Wieland [23]. For each edge on the dual lattice, there is a value for the winding function $w(e)$ at that edge such that the winding angle at the neighboring edge e' is defined by $w(e') = w(e) + \text{the turning angle from } e \text{ to } e' \text{ measured in radians}$. It is shown that the variance of the winding angles, grows with the sample size like

$$\langle \theta^2 \rangle = a + \frac{\kappa}{4} \ln(L). \quad (10)$$

Thus, by plotting $\langle \theta^2 \rangle$ versus $\ln(L)$, the slope gives a direct measure of κ [23].

The finite-size scaling of the spanning cluster size, is of the form [24]

$$M(L) = L^{D_c} \tilde{M}(L/\xi) \quad (11)$$

where the correlation length, also known as the connectedness length, behaves like $\xi \sim (T - T_c)^{-\nu_G}$, and the scaling function $\tilde{M}(x)$ tends to a constant as its argument goes to zero at T_c . Thus, the correlation length exponent ν_G of the geometrical clusters, is estimated by a value that results in a data collapse in a scaling plot $L^{-D_c} M(L)$ against $L^{1/\nu_G}(\beta/\beta_c - 1)$. Among other percolation quantities of interest is the percolation strength $P_\infty(L) = M(L)/L^2$, which is the probability that a site chosen at random belongs to the spanning cluster [24]. P_∞ plays the role of an order parameter for the

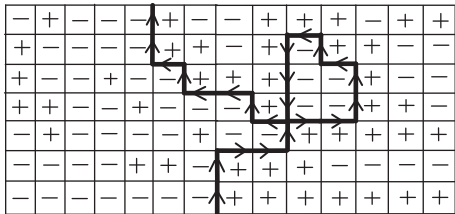


Figure 2. An schematic illustration of defining the domain boundaries in two-dimensional TBIM, on a square lattice. Figure shows the dual of the original square lattice including a spin configuration, with fixed boundary conditions for the bottom end, antiperiodic on sides, and free for the top end. The non-intersecting interface (shown by arrows) is generated using a turn right tie-breaking rule.

percolation transition, and vanishes at the percolation threshold $p_c = \tanh \beta_c$, at a rate specified by an exponent β_G defined by $P_\infty \propto (p - p_c)^{\beta_G}$. The finite-size scaling relation for the strength of percolation, is as follows [24]:

$$P_\infty(L) = L^{-\beta_G/\nu_G} \tilde{P}(L/\xi). \quad (12)$$

Thus, at the critical point T_c , a log-log plot of P_∞ against L must be a straight line with a slope equal to the ratio $-\beta_G/\nu_G$. In the next section, we present our results for the two-dimensional TBIM.

4. Results and discussion

In this section we present and discuss our main results for the two-dimensional TBIM as obtained from simulations based on the methods pointed out in the previous section. We performed simulations for eight different system sizes $L = 100, 150, 200, 250, 300, 350, 400$, and 450 . Only the spin configurations including a vertical spanning cluster are considered for analysis, and the statistical errors were estimated by means of binning the accumulated data. As it appears in figure 3, the slope of a log-log plot of the spanning length l versus the system size L , results in a fractal dimension $D_I = 1.373(8)$, which is equivalent to a $\kappa = 2.984(17)$ as given by equation (8).

To confirm our results, we also measured the winding angle variance along the spanning contour by performing simulations for 10 different system sizes $L = 30, 50, 100, 150, 200, 250, 300, 350, 400$, and 450 . A plot of $\langle \theta^2 \rangle$ against L is shown in figure 4. A curve of the form $a_1 + a_2 \ln(L)$ with parameters $a_1 = -1.330(10)$ and $a_2 = 0.751(2)$ (where $a_2 = \frac{\kappa}{4}$), was least-squares fitted to these data. Furthermore, plotting $\langle \theta^2 \rangle$ versus $\ln(L)$, results in a SLE parameter $\kappa = 3.004(9)$ as illustrated in the inset of figure 4.

A log-log plot of the spanning cluster mass M versus the system size L is shown in figure 5. The slope gives a fractal dimension $D_c = 1.948(3)$.

Using the finite-size scaling ansatz as given in equation (11), the correlation length exponent ν_G for the emerging spanning cluster, is estimated from a scaling plot of

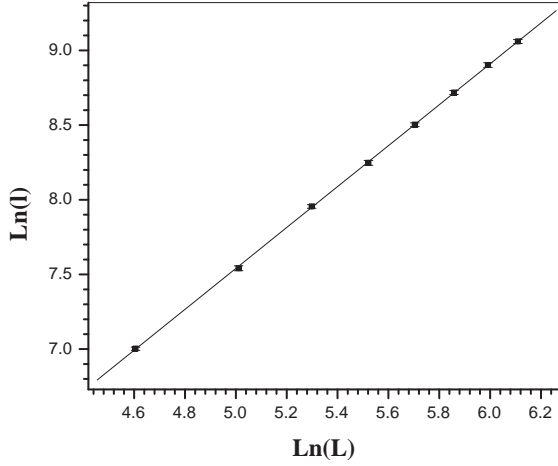


Figure 3. A log-log plot of l against L for the two-dimensional TBIM. The slope of the straight line gives the fractal dimension of the external perimeters $D_I = 1.373(8)$. The error bars are smaller or comparable with the symbol size.

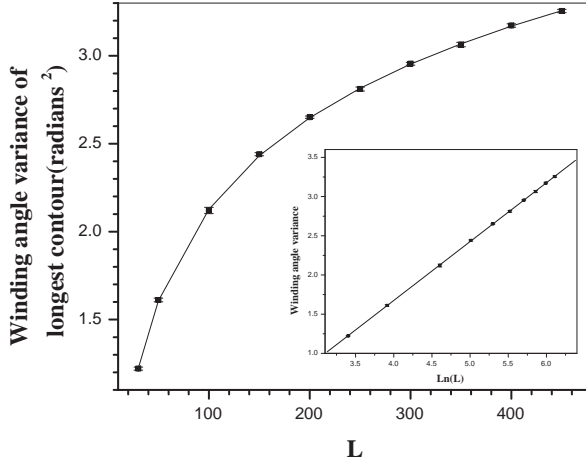


Figure 4. A plot of $\langle \theta^2 \rangle$ versus L for the two-dimensional TBIM. In the inset, the variance is in semi-logarithmic coordinates. The error bars are smaller or comparable with the symbol size.

$L^{-D_c} M(L)$ against $L^{1/\nu_G} (\beta/\beta_c - 1)$ as shown in figure 6. By varying ν_G , and evaluating the quality of the data collapse, our best estimate of the correlation length exponent for the geometrical clusters is $\nu_G = 1.01(2)$. Finally, the slope of the log-log plot of P_∞ versus L results in $\beta_G = 0.051(3)$, as shown in figure 7, which fits well into the hyperscaling relation for the percolation exponents in d spatial dimensions $D_c = d - \frac{\beta_G}{\nu_G}$.

The obtained results for the two-dimensional TBIM are listed in table 1 for comparison with the analytical results of the regular Ising model. At criticality, the fractal dimension of the spin clusters D_c and interfaces D_I have been found to be

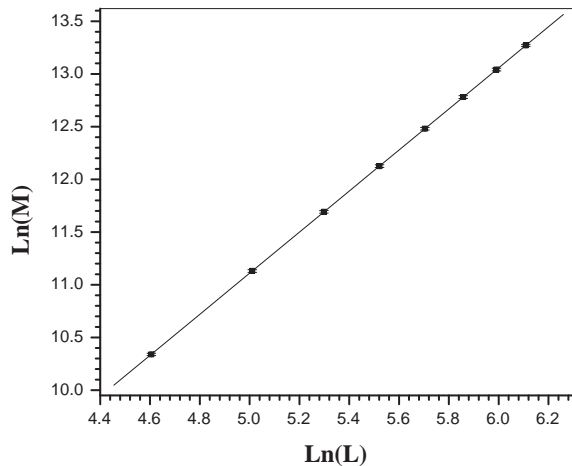


Figure 5. A log-log plot of M against L . The slope of the straight line gives the fractal dimension of the geometrical clusters at T_c , $D_c = 1.948(3)$.

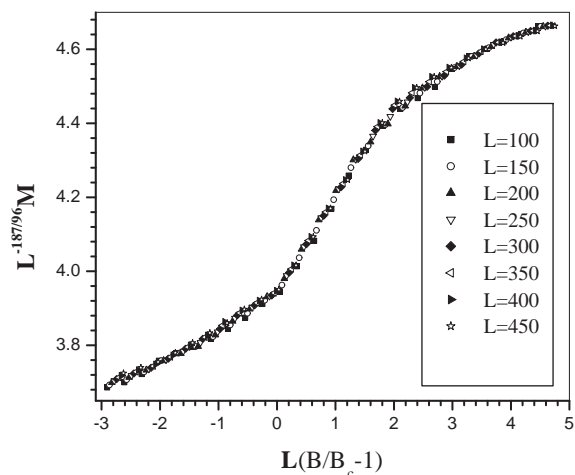


Figure 6. A scaling plot for the spanning cluster mass. By varying ν_G , and evaluating the quality of the data collapse, our best estimate of the correlation length exponent is $\nu_G = 1.01(2)$

Table 1. The critical exponents of the geometrical clusters in 2d TBIM are compared with those obtained for 2d regular Ising model.

	ν_G	β_G	κ	D_I	D_c
TBIM	1.01(2)	0.051(3)	3.004(9)	1.373(8)	1.948(3)
Ising Model	1.00	5/96	3	1.375	187/96

consistent with the analytical results obtained for the regular Ising model, despite the temperature-dependent annealed bond dilution.

It must be noted that although the geometrical clusters (i.e., the neighboring sites

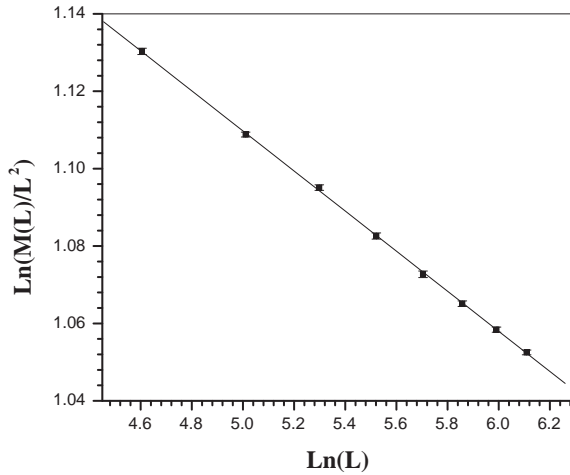


Figure 7. A log-log plot of P_∞ against L . The slope of the straight line gives $\beta_G = 0.051(3)$

of the same spin sign) uniquely characterize the universality class of the critical system, they do not, however, represent the critical droplets. Hence, the percolation critical exponents of the geometrical clusters, do not in general coincide with those of the corresponding thermal quantities. The critical droplets, are more precisely specified by the so-called Fortuin-Kastelyn (FK) clusters whose diffusivity parameter κ has a duality relation with that of the geometric spin clusters [1, 18, 25]. The FK clusters can be obtained from the geometrical clusters through a random decimation of bonds by a suitable probability, in this case $1 - \tanh(\beta)$, and are therefore less compact. Thus, despite the correlation length exponent $\nu_G = 1$, we note that the geometrical clusters are too compact to represent the critical droplets, and the exponent $\beta_G = 5/96$ differs appreciably from the corresponding thermal exponent $\beta = 1/8$, associated with the vanishing of the magnetization order parameter at T_c . The value of the correlation length (also known as the connectivity length) exponent $\nu_G = 1$, for the geometrical clusters of the two-dimensional TBIM, is in excellent agreement with the values obtained from a real-space renormalization group analysis [1, 7], high-temperature series expansion studies [26], and precision numerical simulations of the geometrical clusters of the standard two-dimensional Ising model [2, 27]. This result, however, opens a question about a near perfect collapse onto a universal function for the same data obtained for the regular Ising model, but with a different exponent $\frac{15}{8}$ [21].

As can be seen from table 1, within the statistical uncertainty, the value of the SLE parameter κ , the fractal dimensions, and the percolation exponents of the geometrical spin clusters of the two-dimensional TBIM, are in excellent agreement with those of the corresponding regular Ising model. These results agree well with an earlier study of the thermodynamic critical behavior of the two-dimensional TBIM, which places the model system in the universality class of the standard two-dimensional Ising model

[19], and the Fisher renormalization relations, which assert that annealed bond dilution can only change the critical exponents if the specific heat exponent α_r of the regular model is positive ($\alpha_r > 0$) [28]. The two-dimensional regular Ising model, however, is characterized by a logarithmic divergence of the specific heat, $\alpha_r = 0$, and the exponents remain unchanged.

As for the fractal behavior of the geometrical clusters away from the criticality, we note that for all temperatures below the transition point $T < T_c$ (or $p > p_c$), D_c must equal the space dimensions $d = 2$, otherwise the percolation strength would vanish in the thermodynamic limit of an infinite lattice. At T_c ($p = p_c$), the geometrical clusters of the two-dimensional TBIM, are fractal with a fractal dimension $D_c = 1.948(3)$ (< 2), thus rendering the percolation strength zero at the critical point, as expected. Hence, one expects the fractal dimension of the geometrical clusters to change discontinuously from $D_c = d = 2$ for $T < T_c$, to $D_c = 1.948(3)$ at T_c . This expectation is validated by the data of reference [21], where the so-called ‘effective’ fractal dimensions undergo a sharp crossover at T_c . We believe that the crossover is a finite-size effect, and a remnant of the discontinuity at T_c in the thermodynamic limit. As for the temperatures above the critical point $T > T_c$, there are no spanning geometrical clusters in the thermodynamic limit and the procedures used here become inapplicable. However, other standard procedures such as the box counting method may be employed to investigate the fractal behavior of the geometrical clusters above T_c and within a region of linear size of the order of the finite correlation length ξ .

5. Summary

The fractal behavior of the geometrical spin clusters, are obtained for the thermalized bond Ising model in two dimensions. For this purpose, a modified Wolff single-cluster Monte Carlo simulation is used to generate equilibrium spin configurations on square lattices in the critical region. The obtained values for the fractal dimensions of the spanning geometrical clusters, D_c , and that of their interfaces, D_I , are in perfect agreement with those reported for the regular Ising model. The variance of the winding angles results in a value $\kappa = 3.004(9)$ for the SLE parameter, thus placing it in the universality class of the regular Ising model. Furthermore, the percolation exponents of the geometrical spin clusters at T_c , are found to be consistent with those reported for the regular Ising model. These consistencies are explained in terms of the Fisher renormalization relations, which express the thermodynamic critical exponents of systems with annealed bond dilution in terms of those of the regular model system.

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